LISTING OF CLAIMS

This Listing of Claims will replace all prior versions, and all prior listings, of claims in this application.

1-22. (canceled)

23. (currently amended) A method for selecting ~~at least one of~~ a ~~plurality of~~ chemical ~~entities~~ entity ~~based on its ability to~~ that associates with all or part of a binding pocket of a molecule or molecular complex, or a homologue of said binding pocket, with a deformation energy not greater than about 10 kcal/mole, wherein the ~~binding pocket is defined by~~ structure coordinates of inosine monophosphate dehydrogenase ("IMPDH") amino acids 68, 69, 93, 273, 274, 275, 276, 277, 303, 322, 324, 325, 326, 327, 328, 330, 331, 332, 333, 334, 337, 339, 340, 364, 413, 414, 415, 416, 420, 439, 440, 441, 442, 469, and 470 according to Figure 1 characterize the binding pocket, ~~or a~~ and wherein the homologue of said binding pocket ~~that~~ has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a) determining structure coordinates of inosine monophosphate dehydrogenase ("IMPDH") amino acids 68, 69, 93, 273, 274, 275, 276, 277, 303, 322, 324, 325, 326, 327, 328, 330, 331, 332, 333, 334, 337, 339, 340, 364, 413, 414, 415, 416, 420, 439, 440, 441, 442, 469, and 470 according to Figure 1 to characterize the binding pocket;

[[a)]] b) employing computational means which utilize all or part of said structure coordinates and structure coordinates of [[a]] the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof~~, wherein said docking utilizes energy minimization~~;

[[b)]] c) quantifying the deformation energy ~~association~~ between the chemical entity and all or part of the binding pocket or homologue thereof;

[[c)]] d) outputting said quantified deformation energy ~~association~~ to a suitable output hardware; and

[[d)]] e) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole ~~at least one of said chemical entities based on said quantified association~~.

24-26. (canceled)

27. (currently amended) ~~The~~ A method ~~according to claim 23,~~ for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex, or a homologue of said binding pocket, with a deformation energy not greater than about 10 kcal/mole, wherein ~~said binding pocket is defined by~~ structure coordinates of IMPDH amino acids 275, 276, 303, 325, 326, 331, 333 and 441 according to Figure 1 characterize the binding pocket, and wherein the homologue of said binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a) determining structure coordinates of IMPDH amino acids 275, 276, 303, 325, 326, 331, 333 and 441 according to Figure 1 to characterize the binding pocket;

b) employing computational means which utilize all or part of said structure coordinates and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

c) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

d) outputting said quantified deformation energy to a suitable output hardware; and

e) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

28. (currently amended) ~~The~~ A method ~~according to claim 23,~~ for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex, or a homologue of said binding pocket, with a deformation energy not greater than about 10 kcal/mole, wherein ~~said binding pocket is defined by~~ structure coordinates of IMPDH amino acids 274, 275, 276, 277, 303, 322, 324, 325, 326, 331, 333, 414, 415, and 441 according to Figure 1 characterize the

binding pocket, and wherein the homologue of said binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a) determining structure coordinates of IMPDH amino acids 274, 275, 276, 277, 303, 322, 324, 325, 326, 331, 333, 414, 415, and 441 according to Figure 1 to characterize the binding pocket;

b) employing computational means which utilize all or part of said structure coordinates and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

c) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

d) outputting said quantified deformation energy to a suitable output hardware; and

e) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

29. (currently amended) A method for selecting ~~at least one of~~ a ~~plurality of~~ chemical entity that ~~entities based on its ability to~~ associates with all or part of a binding pocket of a molecule or molecular complex, or a homologue of said binding pocket, with a deformation energy not greater than about 10 kcal/mole, wherein the ~~binding pocket is defined by~~ structure coordinates of inosine monophosphate dehydrogenase ("IMPDH") amino acids 67, 68, 69, 70, 73, 274, 275, 276, 303, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 364, 365, 366, 367, 368, 385, 386, 387, 388, 389, 391, 411, 412, 413, 414, 415, 416, 419, 440, 441, 442, 443, 500, 501, 502, 503, 504, 505, and 506 according to Figure 1 characterize the binding pocket, ~~or a~~ and wherein the homologue of said binding pocket ~~that~~ has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a) determining structure coordinates of inosine monophosphate dehydrogenase ("IMPDH") amino acids 67, 68, 69, 70, 73, 274, 275, 276, 303, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 364, 365, 366, 367, 368, 385, 386, 387, 388, 389, 391, 411, 412, 413, 414, 415, 416, 419, 440, 441, 442,

443, 500, 501, 502, 503, 504, 505, and 506 according to Figure 1 to characterize the binding pocket;

[[a)]] b) employing computational means which utilize all or part of said structure coordinates and structure coordinates of [[a]] the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof~~, wherein said docking utilizes energy minimization~~;

[[b)]] c) quantifying the deformation energy ~~association~~ between the chemical entity and all or part of the binding pocket or homologue thereof;

[[c)]] d) outputting said quantified deformation energy ~~association~~ to a suitable output hardware; and

[[d)]] e) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole ~~at least one of said chemical entities based on said quantified association~~.

30. (currently amended) ~~The~~ A method ~~according to claim 29,~~ for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex, or a homologue of said binding pocket, with a deformation energy not greater than about 10 kcal/mole, wherein ~~said binding pocket is defined by~~ structure coordinates of IMPDH amino acids 68, 70, 322, 328, 329, 331, 332, 335, 364, 366, 387, 388, 411, 413, 414, 415, 441, 442, 501, and 502 according to Figure 1 characterize the binding pocket, and wherein the homologue of said binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a) determining structure coordinates of IMPDH amino acids 68, 70, 322, 328, 329, 331, 332, 335, 364, 366, 387, 388, 411, 413, 414, 415, 441, 442, 501, and 502 according to Figure 1 to characterize the binding pocket;

b) employing computational means which utilize all or part of said structure coordinates and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

c) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

d) outputting said quantified deformation energy to a suitable output hardware; and

e) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

31. (currently amended) ~~The~~ A method ~~according to claim 29,~~ for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex, or a homologue of said binding pocket, with a deformation energy not greater than about 10 kcal/mole, wherein ~~said binding pocket is defined by~~ structure coordinates of IMPDH amino acids 68, 69, 70, 303, 322, 326, 327, 328, 329, 330, 331, 332, 333, 335, 364, 365, 366, 367, 385, 386, 387, 388, 411, 413, 414, 415, 416, 419, 441, 442, 443, 501, 502, 503, and 504 according to Figure 1 characterize the binding pocket, and wherein the homologue of said binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å comprising the steps of:

a) determining structure coordinates of IMPDH amino acids 68, 69, 70, 303, 322, 326, 327, 328, 329, 330, 331, 332, 333, 335, 364, 365, 366, 367, 385, 386, 387, 388, 411, 413, 414, 415, 416, 419, 441, 442, 443, 501, 502, 503, and 504 according to Figure 1 to characterize the binding pocket;

b) employing computational means which utilize all or part of said structure coordinates and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

c) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

d) outputting said quantified deformation energy to a suitable output hardware; and

e) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

32. (currently amended) A method for selecting ~~at least one of~~ a ~~plurality of~~ chemical entity that ~~entities based on its ability to~~ associates with all or part of a binding pocket of a molecule or molecular complex, or a homologue of said binding pocket, with a deformation energy not greater than about 10 kcal/mole, wherein the ~~binding pocket is defined by~~ structure coordinates of inosine monophosphate dehydrogenase ("IMPDH") amino acids 67, 68, 69, 70, 73, 93, 273,

274, 275, 276, 277, 303, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 337, 339, 340, 364, 365, 366, 367, 368, 385, 386, 387, 388, 389, 391, 411, 412, 413, 414, 415, 416, 419, 420, 439, 440, 441, 442, 443, 469, 470, 500, 501, 502, 503, 504, 505, and 506 according to Figure 1 characterize the binding pocket, ~~or a~~ and wherein the homologue of said binding pocket ~~that~~ has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a) determining structure coordinates of inosine monophosphate dehydrogenase ("IMPDH") amino acids 67, 68, 69, 70, 73, 93, 273, 274, 275, 276, 277, 303, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 337, 339, 340, 364, 365, 366, 367, 368, 385, 386, 387, 388, 389, 391, 411, 412, 413, 414, 415, 416, 419, 420, 439, 440, 441, 442, 443, 469, 470, 500, 501, 502, 503, 504, 505, and 506 according to Figure 1 to characterize the binding pocket;

[[a)]] b) employing computational means which utilize all or part of said structure coordinates and structure coordinates of [[a]] the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof~~, wherein said docking utilizes energy minimization~~;

[[b)]] c) quantifying the deformation energy ~~association~~ between the chemical entity and all or part of the binding pocket or homologue thereof;

[[c)]] d) outputting said quantified deformation energy ~~association~~ to a suitable output hardware; and

[[d)]] e) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole ~~at least one of said chemical entities based on said quantified association~~.

33. (currently amended) ~~The~~ A method ~~according to claim 32,~~ for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex, or a homologue of said binding pocket, with a deformation energy not greater than about 10 kcal/mole, wherein ~~said binding pocket is defined by~~ structure coordinates of IMPDH amino acids 68, 70, 275, 276, 303, 322, 325, 326, 328, 329, 331, 332, 333, 335, 364, 366, 387, 388, 411, 413, 414, 415, 441, 442, 501, and 502 according to Figure 1 characterize the binding pocket, and wherein

the homologue of said binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å comprising the steps of:

a) determining structure coordinates of IMPDH amino acids 68, 70, 275, 276, 303, 322, 325, 326, 328, 329, 331, 332, 333, 335, 364, 366, 387, 388, 411, 413, 414, 415, 441, 442, 501, and 502 according to Figure 1 to characterize the binding pocket;

b) employing computational means which utilize all or part of said structure coordinates and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

c) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

d) outputting said quantified deformation energy to a suitable output hardware; and

e) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

34. (currently amended) ~~The~~ A method ~~according to claim 32,~~ for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex, or a homologue of said binding pocket, with a deformation energy not greater than about 10 kcal/mole, wherein ~~said binding pocket is defined by~~ structure coordinates of IMPDH amino acids 68, 69, 70, 274, 275, 276, 277, 303, 322, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 335, 364, 365, 366, 367, 385, 386, 387, 388, 411, 413, 414, 415, 416, 441, 442, 443, 501, 502, 503, and 504 according to Figure 1 characterize the binding pocket, and wherein the homologue of said binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å comprising the steps of:

a) determining structure coordinates of IMPDH amino acids 68, 69, 70, 274, 275, 276, 277, 303, 322, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 335, 364, 365, 366, 367, 385, 386, 387, 388, 411, 413, 414, 415, 416, 441, 442, 443, 501, 502, 503, and 504 according to Figure 1 to characterize the binding pocket;

b) employing computational means which utilize all or part of said structure coordinates and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

c) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

d) outputting said quantified deformation energy to a suitable output hardware; and

e) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

35. (currently amended) ~~The~~ A method for selecting a chemical entity that associates with all or part of a molecule, molecular complex or homologue thereof, with a deformation energy not greater than about 10 kcal/mole ~~according to claim 32~~, wherein said molecule is defined by the set of structure coordinates of IMPDH amino acids according to Figure 1, and said molecular complex is defined by the set of structure coordinates of IMPDH amino acids and ~~one or more of~~ oxidized inosine monophosphate thioimidate intermediate (XMP*) ~~and~~ or mycophenolic acid (MPA) according to Figure 1, and ~~or a homologue thereof, wherein~~ said homologue has a root mean square deviation from the backbone atoms of said IMPDH amino acids of not more than 1.5 Å, comprising the steps of:

a) producing a crystal of said molecule or molecular complex;

b) determining the three-dimensional structure coordinates of the molecule or molecular complex by X-ray diffraction of the crystal;

c) employing computational means which utilize all or part of said structure coordinates and structure coordinates of a chemical entity to dock the chemical entity with all or part of said molecule, molecular complex, or homologue thereof;

d) quantifying the deformation energy between the chemical entity and all or part of the molecule, molecular complex, or homologue thereof;

e) outputting said quantified deformation energy to a suitable output hardware; and

f) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

36. (canceled).

37. (currently amended) The method of claim 32, wherein the docking of the chemical entity with all or part of the binding pocket utilizes shape complementarity or is followed by molecular dynamics or energy minimization.

38. (currently amended) The method according to any one of claims 23, 29 or 32, further comprising the steps of:

e) contacting the selected chemical entity with the molecule or molecular complex; and

f) ~~monitoring~~ selecting the chemical entity that inhibits the catalytic activity of the molecule or molecular complex.

39. (currently amended) ~~The~~ A method for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex with a deformation energy not greater than about 10 kcal/mole, ~~of any one of claims 23, 29 and 32, prior to step a), further~~ comprising the steps of:

a) producing a crystal of a molecule or molecular complex comprising IMPDH;

b) determining the three-dimensional structure coordinates of the molecule or molecular complex by X-ray diffraction of the crystal; ~~and~~

c) employing computational means which utilize all or part of a binding pocket characterized by structure coordinates of inosine monophosphate dehydrogenase ("IMPDH") amino acids S68, P69, H93, L273, D274, S275, S276, Q277, N303, R322, G324, M325, G326, C327, G328, I330, C331, I332, T333, Q334, L337, C339, G340, D364, G413, M414, G415, S416, M420, V439, A440, Q441, G442, Q469, and D470 and structure coordinates of a chemical entity, to dock the chemical entity with all or part of said binding pocket ~~identifying said binding pocket~~;

d) quantifying the deformation energy between the chemical entity and all or part of the binding pocket;

e) outputting said quantified deformation energy to a suitable output hardware; and

f) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

40. (currently amended) The method of claim 32, wherein the docking of the chemical entity with all or part of the binding pocket includes ~~is performed through~~ visual inspection on a computer screen using a computer program capable of generating a three-dimensional graphical representation of said structure coordinates and structure coordinates of said chemical entity.

41. (withdrawn) The method according to claim 23, 27 or 28, further comprising the steps of:

e) repeating steps a) to d) with a second ~~set of a plurality of~~ chemical ~~entities~~ entity that associates with all or another part of said binding pocket, or homologue thereof;

f) optionally, visually inspecting the relationship of the selected first and second chemical entity to each other in relation to the binding pocket or homologue thereof on a computer screen using the three-dimensional graphical representation of the binding pocket or homologue thereof and said selected first and second chemical entity; and

g) assembling the selected first and second chemical entity into a compound or complex that associates with all or part of said binding pocket or homologue thereof by model building.

42 and 43. (canceled).

44. (withdrawn) The method according to claim 29, 30 or 31, further comprising the steps of:

e) repeating steps a) to d) with a second ~~set of a plurality of~~ chemical ~~entities~~ entity that associates with all or another part of said binding pocket, or homologue thereof;

f) optionally, visually inspecting the relationship of the selected first and second chemical entity to each other in relation to the binding pocket or homologue thereof on a computer screen using the three-dimensional graphical representation of the binding pocket or homologue thereof and said selected first and second chemical entity; and

g) assembling the selected first and second chemical entity into a compound or complex that associates with all or part of said binding pocket or homologue thereof by model building.

45 and 46. (canceled).

47. (withdrawn) The method according to claim 32, 33 or 34, further comprising the steps of:

e) repeating steps a) to d) with a second ~~set of a plurality of~~ chemical ~~entities~~ entity that associates with all or another part of said binding pocket, or homologue thereof;

f) optionally, visually inspecting the relationship of the selected first and second chemical entity to each other in relation to the binding pocket or homologue thereof on a computer screen using the three-dimensional graphical representation of the binding pocket or homologue thereof and said selected first and second chemical entity; and

g) assembling the selected first and second chemical entity into a compound or complex that associates with all or part of said binding pocket or homologue thereof by model building.

48 and 49. (canceled).

50. (withdrawn) The method according to claim 35, further comprising the steps of :

e) repeating steps a) to d) with a second ~~set of a plurality of~~ chemical ~~entities~~ entity that associates with all or another part of said molecule, ~~or~~ molecular complex, or homologue thereof;

f) optionally, visually inspecting the relationship of the selected first and second chemical entity to each other in relation to the molecule, molecular complex or homologue thereof on a computer screen using the three-dimensional graphical representation of the molecule, molecular complex or homologue thereof and said selected first and second chemical entity; and

g) assembling the selected first and second chemical entity into a compound or complex that associates with all or part of said molecule, molecular complex or homologue thereof by model building.

51. (withdrawn) The method according to claim 36, further comprising the steps of :

e) repeating steps a) to d) with a second ~~set of a plurality of~~ chemical ~~entities~~ entity that associates with all or another part of said ~~molecule or~~ molecular complex;

f) optionally, visually inspecting the relationship of the selected first and second chemical entity to each other in relation to the ~~molecule,~~ molecular complex ~~or homologue thereof~~ on a computer screen using the three-dimensional graphical representation of the ~~molecule,~~ molecular complex ~~or homologue thereof~~ and said selected first and second chemical entity; and

g) assembling the selected first and second chemical entity into a compound or complex that associates with all or part of said ~~molecule,~~ molecular complex ~~or homologue thereof~~ by model building.

52-62. (canceled).

63. (new) The method of any one of claims 23, 29, 32 and 35 wherein the method is for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex with a deformation energy not greater than about 7 kcal/mole and step d) comprises selecting the chemical entity if said deformation energy is not greater than 7 kcal/mole.

64. (new) A method for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex with a deformation energy not greater than about 10 kcal/mole, comprising the steps of:

a) producing a crystal of a molecule or molecular complex comprising IMPDH;

b) determining the three-dimensional structure coordinates of the molecule or molecular complex by X-ray diffraction of the crystal;

c) employing computational means which utilize all or part of a binding pocket characterized by structure coordinates of inosine monophosphate dehydrogenase ("IMPDH") amino acids S67, S68, P69, M70, V73, D274, S275, S276, N303, R322, V323, G324, M325, G326, C327, G328, S329, I330, C331, I332, T333, Q334, E335, D364, G365, G366, I367, Q368, M385, M386, G387, S388, L389, A391, Y411, R412, G413, M414, G415, S416, A419, A440, Q441, G442, V443, E500, G501, G502, V503, H504, S505, and L506 and structure coordinates of a chemical entity, to dock the chemical entity with all or part of said binding pocket;

d) quantifying the deformation energy between the chemical entity and all or part of the binding pocket;

e) outputting said quantified deformation energy to a suitable output hardware; and

f) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

65. (new) A method for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex with a deformation energy not greater than about 10 kcal/mole, comprising the steps of:

a) producing a crystal of a molecule or molecular complex comprising IMPDH;

b) determining the three-dimensional structure coordinates of the molecule or molecular complex by X-ray diffraction of the crystal;

c) employing computational means which utilize all or part of a binding pocket characterized by structure coordinates of inosine monophosphate dehydrogenase ("IMPDH") amino acids S67, S68, P69, M70, V73, H93, L273, D274, S275, S276, Q277, N303, R322, V323, G324, M325, G326, C327, G328, S329, I330, C331, I332, T333, Q334, E335, L337, C339, G340, D364, G365, G366, I367, Q368, M385, M386, G387, S388, L389, A391, Y411, R412, G413, M414, G415, S416, A419, M420, V439, A440, Q441, G442, V443, Q469, D470, E500, G501, G502, V503, H504, S505, and L506 and structure coordinates of a chemical entity, to dock the chemical entity with all or part of said binding pocket;

d) quantifying the deformation energy between the chemical entity and all or part of the binding pocket;

e) outputting said quantified deformation energy to a suitable output hardware; and

f) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

66. (new) A method for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex with a deformation energy not greater than about 10 kcal/mole, comprising the steps of:

a) producing a crystal of a molecule or molecular complex comprising IMPDH;

b) determining the three-dimensional structure coordinates of the molecule or molecular complex by X-ray diffraction of the crystal;

c) employing computational means which utilize all or part of a binding pocket characterized by structure coordinates of inosine monophosphate dehydrogenase ("IMPDH") amino acids S275, S276, N303, M325, G326, C331, T333 and Q441 and structure coordinates of a chemical entity, to dock the chemical entity with all or part of said binding pocket;

d) quantifying the deformation energy between the chemical entity and all or part of the binding pocket;

e) outputting said quantified deformation energy to a suitable output hardware; and

f) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

67. (new) A method for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex with a deformation energy not greater than about 10 kcal/mole, comprising the steps of:

a) producing a crystal of a molecule or molecular complex comprising IMPDH;

b) determining the three-dimensional structure coordinates of the molecule or molecular complex by X-ray diffraction of the crystal;

c) employing computational means which utilize all or part of a binding pocket characterized by structure coordinates of inosine monophosphate dehydrogenase ("IMPDH") amino acids D274, S275, S276, Q277, N303, R322, G324, M325, G326, C331, T333, M414, G415, and Q441 and structure coordinates of a chemical entity, to dock the chemical entity with all or part of said binding pocket;

d) quantifying the deformation energy between the chemical entity and all or part of the binding pocket;

e) outputting said quantified deformation energy to a suitable output hardware; and

f) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

68. (new) A method for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex with a deformation energy not greater than about 10 kcal/mole, comprising the steps of:

a) producing a crystal of a molecule or molecular complex comprising IMPDH;

b) determining the three-dimensional structure coordinates of the molecule or molecular complex by X-ray diffraction of the crystal;

c) employing computational means which utilize all or part of a binding pocket characterized by structure coordinates of inosine monophosphate dehydrogenase ("IMPDH") amino acids S68, M70, R322, G328, S329, C331, I332, E335, D364, G366, G387, S388, Y411, G413, M414, G415, Q441, G442, G501 and G502 and structure coordinates of a chemical entity, to dock the chemical entity with all or part of said binding pocket;

d) quantifying the deformation energy between the chemical entity and all or part of the binding pocket;

e) outputting said quantified deformation energy to a suitable output hardware; and

f) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

69. (new) A method for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex with a deformation energy not greater than about 10 kcal/mole, comprising the steps of:

a) producing a crystal of a molecule or molecular complex comprising IMPDH;

b) determining the three-dimensional structure coordinates of the molecule or molecular complex by X-ray diffraction of the crystal;

c) employing computational means which utilize all or part of a binding pocket characterized by structure coordinates of inosine monophosphate dehydrogenase ("IMPDH") amino acids S68, P69, M70, N303, R322, G326, C327, G328, S329, I330, C331, I332, T333, E335, D364, G365, G366, I367, M385, M386, G387, S388, Y411, G413, M414, G415, S416, A419, Q441, G442, V443, G501, G502, V503, and H504 and structure coordinates of a chemical entity, to dock the chemical entity with all or part of said binding pocket;

d) quantifying the deformation energy between the chemical entity and all or part of the binding pocket;

e) outputting said quantified deformation energy to a suitable output hardware; and

f) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

70. (new) A method for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex with a deformation energy not greater than about 10 kcal/mole, comprising the steps of:

a) producing a crystal of a molecule or molecular complex comprising IMPDH;

b) determining the three-dimensional structure coordinates of the molecule or molecular complex by X-ray diffraction of the crystal;

c) employing computational means which utilize all or part of a binding pocket characterized by structure coordinates of inosine monophosphate dehydrogenase ("IMPDH") amino acids S68, M70, S275, S276, N303, R322, M325, G326, G328, S329, C331, I332, T333, E335, D364, G366, G387, S388, Y411, G413,

M414, G415, Q441, G442, G501 and G502 and structure coordinates of a chemical entity, to dock the chemical entity with all or part of said binding pocket;

d) quantifying the deformation energy between the chemical entity and all or part of the binding pocket;

e) outputting said quantified deformation energy to a suitable output hardware; and

f) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

71. (new) A method for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex with a deformation energy not greater than about 10 kcal/mole, comprising the steps of:

a) producing a crystal of a molecule or molecular complex comprising IMPDH;

b) determining the three-dimensional structure coordinates of the molecule or molecular complex by X-ray diffraction of the crystal;

c) employing computational means which utilize all or part of a binding pocket characterized by structure coordinates of inosine monophosphate dehydrogenase ("IMPDH") amino acids S68, P69, M70, D274, S275, S276, Q277, N303, R322, G324, M325, G326, C327, G328, S329, I330, C331, I332, T333, E335, D364, G365, G366, I367, M385, M386, G387, S388, Y411, G413, M414, G415, S416, Q441, G442, V443, G501, G502, V503, and H504 and structure coordinates of a chemical entity, to dock the chemical entity with all or part of said binding pocket;

d) quantifying the deformation energy between the chemical entity and all or part of the binding pocket;

e) outputting said quantified deformation energy to a suitable output hardware; and

f) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.